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Project/Task ISV Code Implementation
Subtask Modeling Requirements for ISV

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Subject : Outline of Modeling Requirements for In Situ Vitrification

This document defines the basic requirements for the development of a mathematical representation and computer model of the In Situ Vitrification (ISV) process. These requirements are defined in terms of model capabilities, ISV process variables and input parameters, and waste forms to be remediated. The purpose of this modeling effort is to create a tool which can be used to predict ISV process emissions and performance, and to define an operating envelope for the range of waste forms and dispositions present at INEL burial sites.

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OUTLINE OF MODELING REQUIREMENTS FOR IN SITU VITRIFICATION

I. Purpose

This document defines the basic requirements for the development of a mathematical representation and computer model of the In Situ Vitrification (ISV) process. These requirements are defined in terms of model capabilities, ISV process variables and input parameters, and waste forms to be remediated. The purpose of this modeling effort is to create a tool which can be used to predict ISV process emissions and performance, and to define an operating envelope for the range of waste forms and dispositions present at INEL burial sites.

II. Modeling Requirements

The ISV model will be used to perform the following tasks:

1. Predict composition and distribution of radionuclides within the melt zone so that criticality can be assessed.

2. Estimate ISV process emissions for:
   a. Predicting a range of duration, quantity, and composition of the off-gas.
   b. Provide data on proposed scenarios for preparing an emergency air pollution episode plan, and testing emergency response and process shut-down procedures.
   c. Performing site-specific air quality hazard assessments to determine potential worker and local population health effects during and after remediation.
   d. Performing sensitivity analyses for assumptions and uncertainties used in hazard assessments.
   e. Determining performance requirements for the off-gas collection and treatment system.

3. Determining subsurface vapor and entrained particulate migration beyond the vitrified zone during and after remediation.

4. Identify and quantify uncertainties, and hence risk, associated with ISV process implementation. The uncertainties arise due to statistical variations in soil and waste material properties, imprecise knowledge of waste forms and dispositions, equipment failure, and operator errors.

5. Identify the parameters and conditions controlling the process for:
   a. Determining the effects of soil properties and waste composition on melt zone growth rates and geometries;
   b. Determining the effects of operator controlled parameters on growth rates and geometries;
   c. Estimating energy consumption per unit mass of vitrified soil;
   d. Estimating time required to complete the process.

6. Predict composition and distribution of hazardous materials in the vitrified matrix so that product leachability and durability can be assessed.

7. Predict long term deformation (creep) characteristics of the vitrified matrix.

III. Phenomena to be Modeled

The mathematical model is to be based on a reasonably fundamental description of the important physical phenomena occurring during and after vitrification. These phenomena include:

1. Thermochemical and electrochemical reaction kinetics and stoichiometry
2. Transport of gases and particulates in the melt zone and surrounding porous media
3. Convective mixing and buoyancy effects in the melt zone
4. Heat transfer with phase change
5. Electric heating
6. Nonlinear and anisotropic material properties
7. Variations in power system operations.

IV. Parameters to be Estimated

The foregoing tasks require that the following parameters be estimated:

1. Three-dimensional geometry and growth rates of the melting zone;
2. Composition and quantity of off-gas generation from the melt zone;
3. Temperature, composition, and combustion behavior of off-gases in the containment hood;
4. Transport of gases in the melt zone and surrounding soil;
5. Distribution and composition of hazardous substances in the vitrified zone and surrounding soil;
6. In situ temperature field during and after remediation;
7. Electric potential field and heat generation in the melt zone;
8. Viscous flow field within the melt zone and the transport of waste by convection;
9. Long-term time dependent deformation and waste migration in the vitrified matrix.

V. Model Input Parameters

A primary reason for creating the model is to identify the important parameters controlling the ISV process. Therefore, the parameters listed below represent only some of the parameters which must be user defined. Other parameters which are important to the simulation will be identified during model development. Moreover, statistical variations in these parameters are important and will be quantified.

1. Power System Variables
    a. Voltage and current input
    b. Electrode spacing
    c. Electrode depth versus time or melt depth
    d. Electrode oxidation rates

2. Effective Physical Properties of Soil and Waste
    a. Electrical conductivities
    b. Moisture contents
    c. Porosity and permeability
    d. Thermal conductivities and heat capacities
    e. Densities
    f. Viscosity of molten soil
    g. Heat of fusion and fusion temperatures
    h. Thermic and kinetic reaction parameters for waste volatilization.

VI. <u>Waste Forms</u>

Since a wide range of waste forms and dispositions are to be remediated, the model must allow for variations in:

1. Chemical composition and volume of waste
2. Initial in situ distribution and configuration
3. Sealed containers with void volumes
4. Buried inclusions such as metals and ceramics.

VII. <u>Software Design and Specifications</u>

The ISV computer code will be written in Standard FORTRAN 77. Software design practices employed in code development and documentation will result in a product that is modular, easily maintainable, and portable. To reduce computational costs, workstations and personal computers will be used for code development.

User friendly code-interface features will include:

a. Checkpoint and restart capability
b. Free format data entry and extraction
c. Interactive (window/graphical/mouse based) entry of initialization and restart data
d. One line time step summary
e. Dynamic (window/graphical/mouse based) summary of time-dependent information
f. Command mode input which allows the user to specify the sequence of operations required to execute the problem in batch mode
g. Interactive execution of the problem using a workstation to interface to the user, and a supercomputer as a user-transparent computer server
h. For testing purposes, the ability for a user to specify an alternate user-transparent computer server
i. Conformance to all applicable interface standards (OPEN-LOOK, MOTIF, GKS, PHIGS, X-Windows, SUNRPC, etc.).

In selecting a numerical discretization method to solve the mathematical system of equations representing the ISV process, the following basic guidelines will be adhered to:

1. Since many of the vitrification processes are three dimensional in nature, the model must be applicable to two-and-three dimensional analyses.

2. The numerical methods must be suitably general to allow model improvements and modifications without requiring the basic code structure and solution schemes to be changed.
3. The structure and linking of the major model components, and the logic controlling module calls, will be designed to accommodate a step-by-step growth of the code and its components.
4. Specific requirements for each modeling task will be defined prior to its development.

VIII. Interactive Output and Postprocessing Capabilities

The computer model will permit easy interpretation and utilization of computer simulation results. The user may elect to output, in tabular or graphical form, a number of transient fieldwide quantities including:

1. Melt zone growth rates and geometries
2. Energy consumption
3. Composition and quality of off-gases
4. Power consumption and energy losses
5. Viscous flow and temperature fields
6. Waste disposition during and after remediation.

IX. Validation Requirements

Validation of the ISV model will be a continuing process as the laboratory and field test efforts progress. Validation efforts will utilize INEL experimental data and data from other research programs.

The inherent limitations of the mathematical model and uncertainties in the approximate model calculations will be assessed. The numerical methods involved will be tested for stability, convergence, and accuracy. Accuracy of the various ISV model components will be evaluated using exact and proved approximate solutions to appropriate model problems. All model components will be fully tested in isolation.

X. Milestones and Schedule

1. Short-term Milestones

   a. Draft of the Requirements Document (11/15/89)
   b. Implementation Plan (01/15/90)
   c. Letter summarizing peer review (04/15/90)
   d. Completed Verification Plan (07/15/90)
   e. Completed Data Requirements Document (09/30/90)
   f. First component of the ISV computer model (09/30/90)
   g. Completion reports on the first components of the ISV computer model (09/30/90)

2. Long-term Milestones (to be determined).